

CLAIMS

1. A method of comparing molecules, comprising:
providing a set of field points representing field extrema of a first molecule,
wherein each field point has a position and a field size value;
5 determining at the position of each of the field points of the first molecule the
field of a second molecule to obtain a set of field sample values; and
combining the field sample values with the field size values to obtain a score
indicative of the field similarity of the first molecule to the second molecule.
- 10 2. The method of claim 1, wherein the field sample values are determined by
applying the position of each of the field points to a field definition formula.
3. The method of claim 1, wherein the field sample values are determined by
calculating the fields by interpolation from a pre-calculated grid of field size values
15 around the second molecule.
4. The method of any preceding claim, wherein, during the combining, the field
size values are transformed to scaled field size values such that two field points
having a first field size value give the same contribution to the score as one field point
20 having a field size value twice the first field size value.
5. The method of claim 4, wherein the scaled field size values have the
magnitude of the square root of the absolute field size values and the sign of the field
size values.
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6. The method of any preceding claim, wherein comparing the field sample
values and the field size values involves obtaining their product.
7. The method of any preceding claim, further comprising:

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providing a set of field points representing field extrema of the second molecule, wherein each field point has a position and a field size value;

determining at the position of each of the field points of the second set the field of the first molecule to obtain a further set of field sample values;

5 combining the further field sample values with the field size values of the field points of the second set to obtain a further score, wherein the further score is indicative of the field similarity of the second molecule to the first molecule; and

combining the further score with the score of the field similarity of the first molecule to the second molecule to obtain an aggregate score.

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8. The method of claim 7, wherein the further field sample values are determined by applying the position of each of the field points of the second set to a field definition formula.

15 9. The method of claim 7, wherein the further field sample values are determined by calculating the fields by interpolation from a pre-calculated grid of field size values around the first molecule.

10. The method of any of claims 7 to 9, wherein comparing the further field sample values and the field size values involves obtaining their product.

11. The method of any preceding claim, wherein the field size values are energy values.

25 12. The method of any preceding claim, wherein the field extrema are field minima.

13. A computer interpretable medium bearing a set of instructions for carrying out the process of any one of the preceding claims.

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14. A computer interpretable medium according to claim 13, wherein the computer interpretable medium is a signal carrier medium.

15. A computer interpretable medium according to claim 13, wherein the
5 computer interpretable medium is a recording medium.

16. A computer apparatus configured to carry out the method of any one of claims
1 to 12.